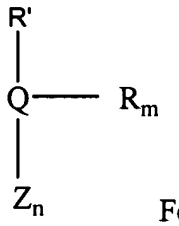
We Claim:

1. A core fragment library comprising a plurality of core fragments, wherein said core fragments have the formula



Formula 1

wherein

Z is a handle capable of anomalous dispersion;

Q is a central core;

Q may be the same or different on each compound;

Each R is, independently, H or a handle;

Each R' is, independently, H or a handle;

n is an integer 0 or greater;

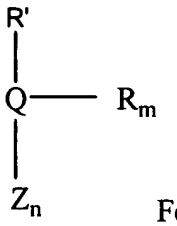
m is an integer 0 or greater; and

(m + n) cannot be greater than the number of available bonds on Q.

2. A mixture comprising a biological target molecule and a plurality of core fragments of the library of claim 1.

3. A mixture comprising a biological target molecule and a library of claim 1.

4. A compound library comprising a plurality of compounds, wherein said compounds have the formula



Formula 1

wherein

Z is a handle capable of anomalous dispersion;

Q is a central core, and for each compound, Q is the same;

Each R is, independently, H or a handle;

Each R' is, independently, H or a derived substituent;

n is an integer 0 or greater; m is an integer 0 or greater; and

(m + n) cannot be greater than the number of available bonds on Q;

with the provisos that

for the majority of compounds in the library, the same R groups are at the same position on Q;

for the majority of compounds in the library, R' is at the same position on Q; and for the majority of compounds in the library, each n is the same.

5. A mixture comprising a biological target molecule and a compound of the library of claim 4.

6. A method of preparing the mixture of claim 5, comprising

a) Obtaining said library; and

b) Preparing a mixture of a compound of said library and a biological target molecule.

7. Processor executable instructions on one or more computer readable storage devices wherein said instructions cause representation and/or manipulation, via a computer output device, of a core fragment library according to claim 1.

8. Processor executable instructions on one or more computer readable storage devices wherein said instructions cause representation and/or manipulation, via a computer output device, of a core fragment library according to claim 4.

9. A core fragment library comprising a plurality of core fragments wherein each of said core fragments comprises:

a) two or more handles; and

b) less than 17 non-hydrogen atoms.

10. The library of claim 9, wherein at least one of said core fragments comprises at least one single or fused ring system.

11. The library of claim 9, wherein at least one of said core fragments comprises at least one heteroatom on at least one ring.

12. The library of claim 9, wherein at least one of said core fragments comprises at least one hetero atom in the central core.

13. The library of claim 9, wherein,

a) at least 50% of the core fragments have less than four hydrogen bond donors;

b) at least 50% of the core fragments have less than four hydrogen bond acceptors; and

c) at least 50% of the core fragments have a calculated LogP value of less than 4.

14. Processor executable instructions on one or more computer readable storage devices wherein said instructions cause representation and/or manipulation, via a computer output device, of a core fragment library according to claim 9.

15. A core fragment library comprising a plurality of core fragments wherein

a) each of said core fragments comprises two or more handles;

b) at least 50% of the core fragments have less than four hydrogen bond donors;

c) at least 50% of the core fragments have less than four hydrogen bond acceptors; and

d) at least 50% of the core fragments have a calculated LogP value of less than 4.

16. Processor executable instructions on one or more computer readable storage devices wherein said instructions cause representation and/or manipulation, via a computer output device, of a core fragment library according to claim 15.

17. A linear compound library comprising a plurality of compounds, wherein each compound comprises

a) the same central core;

b) n handles, wherein said handles are attached at the same positions on each compound; and

c) at least one derived substituent that differs from the derived substituent on another compound of said library;

wherein said derived substituent is derived from one handle and n+1 is an integer and less than or equal to the number of available bonds on the central core.

18. The library of claim 17, wherein said derived substituents on said compounds have been selected using computational methods.

19. The library of claim 18, wherein said derived substituents on said compounds have been selected to have improved biological activity against a biological target molecule.

20. The library of claim 17, wherein said derived substituents have been selected after a screening step, wherein said screening step comprises obtaining the structure of a core fragment in association with a biological target molecule.

21. The library of claim 17, wherein

50% or more of the compounds have a molecular weight of less than about 300 Daltons; and/or

50% or more of the compounds comprise less than about 5 heteroatoms.

22. Processor executable instructions on one or more computer readable storage devices wherein said instructions cause representation and/or manipulation, via a computer output device, of a library according to claim 17.

23. A compound library comprising two or more compound libraries of claim 17.

24. Processor executable instructions on one or more computer readable storage devices wherein said instructions cause representation and/or manipulation, via a computer output device, of a library according to claim 23.

25. A combination of structures for analysis, said combination comprising a library according to claim 1, or a member of said library, and a biological target molecule, wherein said structures comprise member(s) of said library, said target molecule, and combinations thereof.

26. A combination of structures for analysis, said combination comprising a library according to claim 4, or a member of said library, and a biological target molecule, wherein said structures comprise member(s) of said library, said target molecule, and combinations thereof.

27. A combination of structures for analysis, said combination comprising a library according to claim 9, or a member of said library, and a biological target molecule, wherein said structures comprise member(s) of said library, said target molecule, and combinations thereof.

28. A combination of structures for analysis, said combination comprising a library according to claim 15, or a member of said library, and a biological target molecule, wherein said structures comprise member(s) of said library, said target molecule, and combinations thereof.

29. A combination of structures for analysis, said combination comprising a library according to claim 17, or a member of said library, and a biological target molecule, wherein said structures comprise member(s) of said library, said target molecule, and combinations thereof.

30. A combination of structures for analysis, said combination comprising a library according to claim 23, or a member of said library, and a biological target molecule, wherein said structures comprise member(s) of said library, said target molecule, and combinations thereof.

31. A mixture for analysis by x-ray crystallography, said mixture comprising a plurality of core fragments selected from a library according to claim 1 and a biological target molecule.

32. A mixture for analysis by x-ray crystallography, said mixture comprising a plurality of core fragments selected from a library according to claim 9 and a biological target molecule.

33. A mixture for analysis by x-ray crystallography, said mixture comprising a plurality of core fragments selected from a library according to claim 15 and a biological target molecule.

34. A method of designing a lead candidate having activity against a biological target molecule, comprising

a. Obtaining a library of claim 1;

b. Determining the structures of one or more, or at least two, members of said library in association with said biological target molecule; and

c. selecting information from the structure(s) to design at least one lead candidate.

35. The method of claim 34, further comprising the step of determining the structure of said lead candidate in association with said biological target molecule.

36. The method of claim 34, further comprising the step of designing at least one second library of compounds wherein

a) each compound of said second library comprises a central core and two or more handles; and

b) each compound of said second library differs from each other compound of said second library by at least one derived substituent.

37. The method of claim 36, wherein said central core and the central core of said lead candidate are the same.

38. The method of claim 36, further comprising the steps of

Obtaining said second library; and

Determining the structures of one or more, or at least two, compounds of said second library in association with said biological target molecule.

39. The method of claim 34, wherein said biological target molecule is a protein.

40. The method of claim 34, wherein said biological target molecule is a nucleic acid.

41. The method of claim 34, further comprising the steps of
selecting information about said structures to design at least one second library, wherein said second library is derived from at least one core fragment of said core fragment library; and
comprises compounds having modifications on at least one of the handles on said core fragment.

42. A method of designing a lead candidate having activity against a biological target molecule, comprising
a) Obtaining a mixture of claim 2;
b) Determining the structure of at least one core fragment of said mixture in association with said biological target molecule;
c) Selecting information from the structure to design at least one lead candidate.

43. A method of designing a candidate compound having activity against a second biological target molecule, comprising
a) Obtaining a lead candidate by the method of claim 34;
b) Determining the interaction of said lead candidate with a second biological target molecule; and
c) Designing at least one second library of compounds wherein each compound of said second library comprises a central core found in said lead candidate and modifications on at least one of the handles on said central core.

44. A method of designing a core fragment library for drug discovery, comprising screening or reviewing a list of synthetically accessible or commercially available core fragments, and selecting core fragments for said library wherein each of said core fragments comprises:
a) two or more handles; and

b) less than 17 non-hydrogen atoms.

45. A method of screening for a core fragment for use as a base core fragment for library design, comprising

a) Obtaining a library of claim 1;

b) Screening said library for members having binding activity against a biological target molecule; and

c) Selecting a core fragment of member(s) with binding activity to use as a base core fragment for library design.

46. A method of screening for a core fragment for use as a base core fragment for library design, comprising

a) Obtaining a library of claim 9;

b) Screening said library for members having binding activity against a biological target molecule; and

c) Selecting a core fragment of member(s) with binding activity to use as a base core fragment for library design.

47. A method of screening for a core fragment for use as a base core fragment for library design, comprising

a) Obtaining a library of claim 15;

b) Screening said library for members having binding activity against a biological target molecule; and

c) Selecting a core fragment of member(s) with binding activity to use as a base core fragment for library design.

48. A method of identifying a lead candidate having biophysical or biochemical activity against a biological target molecule, comprising

a) Obtaining the structure of said biological target molecule bound to a compound, wherein said compound comprises a first handle having anomalous dispersion properties;

b) Synthesizing a lead candidate molecule comprising the step of replacing said handle on said compound with a second substituent comprising a functionalized carbon, nitrogen, oxygen, or sulfur atom;

c) Assaying said lead candidate molecule for biophysical or biochemical activity against said biological target molecule to identify a lead candidate.

49. The method of claim 48, wherein said second substituent comprises a functionalized carbon or nitrogen atom.

50. A method of designing a lead candidate having biophysical or biochemical activity against a biological target molecule, comprising

a) Combining a biological target molecule with a mixture comprising at least two compounds, wherein at least one of said compounds comprises a substituent having anomalous dispersion properties;

b) Identifying a compound bound to said biological target molecule;

c) Synthesizing a lead candidate molecule comprising the step of replacing said anomalous dispersion substituent with a substituent comprising a functionalized carbon, nitrogen, oxygen, or sulfur atom;

d) Assaying said lead candidate molecule for biophysical or biochemical activity against said biological target molecule.

51. A lead candidate obtained by the method of claim 34.

52. A lead candidate obtained by the method of claim 48.

53. A lead candidate obtained by the method of claim 50.

54. A library obtained by the method of claim 44.

55. A library comprising core fragments selected by the method of claim 47.

56. A candidate compound obtained by the method of claim 43.